Benzenamine, 3,4-dimethyl-

Other names:	1-Amino-3,4-dimethylbenzene
	3,4-Dimethylaminobenzene
	3,4-Dimethylaniline
	3,4-Dimethylbenzenamine
	3,4-Dimethylbenzeneamine
	3,4-Dimethylphenylamine
	3,4-Xylidine
	3,4-Xylylamine
	4-Amino-1,2-dimethylbenzene
	4-Amino-o-xylene
	Aniline, 3,4-dimethyl
	NSC 41800
Inchi:	InChI=1S/C8H11N/c1-6-3-4-8(9)5-7(6)2/h3-5H,9H2,1-2H3
InchiKey:	DOLQYFPDPKPQSS-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	Cc1ccc(N)cc1C
Mol. weight [g/mol]:	121.18
CAS:	95-64-7

Physical Properties

Property code	Value	Unit	Source
gf	176.08	kJ/mol	Joback Method
hf	38.93	kJ/mol	Joback Method
hfus	14.94	kJ/mol	Joback Method
hvap	47.64	kJ/mol	Joback Method
ie	7.68 ± 0.05	eV	NIST Webbook
log10ws	-2.06		Crippen Method
logp	1.886		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
rinpol	201.78		NIST Webbook
rinpol	1173.80		NIST Webbook
rinpol	1173.80		NIST Webbook
rinpol	1177.70		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1196.00		NIST Webbook
ripol	1888.90		NIST Webbook

tb	499.20	K	NIST Webbook
tc	717.26	K	Joback Method
tf	322.10 ± 1.00	K	NIST Webbook
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.80	J/mol×K	491.61	Joback Method
cpg	240.98	J/mol×K	529.22	Joback Method
cpg	252.48	J/mol×K	566.83	Joback Method
cpg	263.33	J/mol×K	604.43	Joback Method
cpg	273.54	J/mol×K	642.04	Joback Method
cpg	283.15	J/mol×K	679.65	Joback Method
cpg	292.16	J/mol×K	717.26	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49973e+01
Coeff. B	-4.34598e+03
Coeff. C	-8.04700e+01
Temperature range (K), min.	375.92
Temperature range (K), max.	529.17

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C95647&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume